Mean-field description of pairing effects, BKT physics, and superfluidity in 2D Bose gases

Chih-Chun Chien,[1] Jianhuang She,[1] and Fred Cooper[1, 2]

[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2]*Santa Fe Institute, Santa Fe, New Mexico 87501, USA*
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We derive a mean-field description for two-dimensional (2D) interacting Bose gases at arbitrary temperatures. We find that genuine Bose-Einstein condensation with long-range coherence only survives at zero temperature. At finite temperatures, many-body pairing effects included in our mean-field theory introduce a finite amplitude for the pairing density, which results in a finite superfluid density. We incorporate Berenzinskii-Kosterlitz-Thouless (BKT) physics into our model by considering the phase fluctuations of our pairing field. This then leads to the result that the superfluid phase is only stable below the BKT temperature due to these phase fluctuations. In the weakly interacting regime at low temperature we compare our theory to previous results from perturbative calculations, renormalization group calculations as well as Monte Carlo simulations. We present a finite-temperature phase diagram of 2D Bose gases. One signature of the finite amplitude of the pairing density field is a two-peak structure in the single-particle spectral function, resembling that of the pseudogap phase in 2D attractive Fermi gases.

I. INTRODUCTION

Recent experiments on two-dimensional (2D) ultra-cold atoms have explored many interesting phenomena including the Berenzinskii-Kosterlitz-Thouless (BKT) physics [1], superfluidity [2], scale invariance [3], radio-frequency (RF) spectroscopy [4], thermodynamics [5], pseudogap physics above the BKT transition temperature [6], and others. These experiments provide opportunities for studying more complicated 2D or layered systems related to high-temperature superconductors [7, 8] and interface superconductivity [9]. Theoretical studies on dilute 2D Bose gases have been reviewed in Ref. [10] and those available theories are confined to weakly interacting regimes or temperatures close to zero or near the critical regime. As a consequence, finite-temperature phase diagrams shown in Ref. [10] are schematic instead of coming from a consistent theoretical description. A mean-field theory that works in the regime of intermediate interaction strength at arbitrary temperature thus would be highly desired for a systematic analysis of 2D interacting Bose gases. To better understand the physics, one needs a coherent description of superfluidity, the BKT transition, pairing effects, and single-particle excitation energy. The goal of this paper is to present a plausible mean-field theory with experimental consequences for a 2D interacting single-species Bose gas.

For an attractive 2D two-component Fermi gas, there have been theories based on the phase fluctuations of the BCS theory and its extension to Bose-Einstein condensation (BEC) of dimers [7, 11]. When the temperature T is below a pairing onset temperature, pairs with disordered phases emerge. When T falls below the BKT transition temperature T_{BKT}, a superfluid phase becomes stable but a genuine long-range ordered phase only survives at $T = 0$. For bosons we may explore similar physics. Several questions follow: How can BKT physics be incorporated into a theory of 2D interacting bosons? Does any interesting phase exist above T_{BKT}? Can 2D bosons have an energy gap in the single-particle excitation? These issues will be addressed in a consistent theoretical framework.

Ref. [10] poses a series of questions that needs to be explored in theoretical work on 2D interacting Bose gases. The last one is "Could one justify a large-N approach which improves on existing methods by incorporating the t-matrix approximation?". Inspired by this question, here we base our theory on the leading-order-auxiliary-field (LOAF) theory of interacting bosons [12, 13], which is a generalization of the conventional large-N expansion [14–16]. It also reduces to the large-N expansion in the normal phase. The LOAF theory is a mean-field theory for interacting Bose gases. Its advantages in describing a 3D Bose gas beyond perturbative regimes at arbitrary temperature are summarized below. In the following we will construct a mean-field theory that applies to 2D Bose gases and explore its thermodynamics and possible experimental implications.

For 3D interacting bosons the LOAF theory meets three important criteria by treating the pairing (anomalous) density field and the (normal) density field on equal footing: (i) a gapless dispersion in the BEC phase, (ii) a conserving theory, and (iii) predicts a second-order BEC transition. Widely used theories such as the Hartree-Fock theory or the Popov theory fail at least one criterion [13]. Moreover, the LOAF theory exhibits a shift in the critical temperature T_c consistent with the results of Ref. [17]. We emphasize that the LOAF theory naturally recovers the Bogoliubov theory of weakly interacting bosons [12] and note that two Green's functions corresponding to our two density fields are indeed present in the Bogoliubov theory [18]. An important feature of the LOAF approximation is that the superfluid density is closely related to the pairing density [19] and the two quantities obey a Josephson relation [20]. This will be crucial in integrating the BKT physics into the LOAF theory of 2D Bose gases.

Before presenting our theory, we point out several challenges in developing a consistent mean-field theory for 2D interacting Bose gases. For 2D systems with short-ranged interactions, Mermin-Wagner theorem [21] rules out the possibility of long-range order. Therefore at finite T a genuine

condensate is not possible in the thermodynamic limit. The lack of a genuine condensate implies that a gapless Goldstone mode may not exist so that the dispersion of excitations should be gapped rather than having the gapless Bogoliubov dispersion relation found in three dimensions in the condensate phase. This challenge may be circumvented by confining the discussion on finite-size patches of the system or introducing phase fluctuations to disorder the condensate [10]. Here we consider 2D Bose gases in the thermodynamic limit so we follow the second approach. The two-body scattering problem in 2D is also very different from that in 3D (see Refs. [10, 22]). The scattering amplitude in 3D is finite as both the energy- and momentum- transfers approach zero. This allows one to develop an effective theory with a coupling constant set equal to the scattering amplitude at zero energy- and momentum-transfer. In contrast, the 2D scattering amplitude vanishes in the limit of zero energy- and momentum- transfer. Following the standard renormalization methods [15], one has to formulate a running coupling constant which should be defined at a finite energy (or momentum) scale. A renormalization scheme for the running coupling constant will be presented and the running coupling constant indeed exhibits behavior consistent with the t-matrix analysis of the scattering amplitude.

This paper is organized as follows. Section II shows the derivation of the 2D LOAF theory. The renormalization of the finite temperature effective potential and the incorporation of phase fluctuations and the BKT physics are addressed in detail. In Section III we present the calculated phase diagram and the experimental implications of the 2D LOAF theory. Comparisons with perturbative calculations are also presented. Section IV states the conclusions of our work.

II. LOAF THEORY OF 2D INTERACTING BOSE GASES

The action of a homogeneous 2D Bose gas is given by $S = \int dx \mathcal{L}$, where $dx \equiv dt d^2x$ and the Lagrangian density is

$$\mathcal{L} = \frac{1}{2}[\phi^*(x)h\phi(x) + \phi(x)h^*\phi^*(x)] - \frac{\lambda}{2}|\phi(x)|^4. \quad (1)$$

Here $h = i\hbar\partial_t + \hbar^2\nabla^2/2m + \mu$ and μ is the chemical potential. We set $\hbar \equiv 1$. λ is the bare 2D repulsive coupling constant. After discussing its renormalization, we will show its connection to the 2D s-wave scattering length. This action is equivalent to the Hamiltonian

$$H = \frac{\hbar^2}{2m}|\nabla\phi|^2 + \frac{\lambda}{2}|\phi|^4. \quad (2)$$

Although the Hamiltonian approach to BECs is more common in the literature, having a path-integral formulation of the problem allows for certain expansion methods that would be hard to implement in the canonical formalism. The expansion used here is one such expansion which allows one to interpret a mean-field theory as the first term in a complete resummation of the original theory by utilizing a Hubbard-Stratonovich transformation [23] and then reversing the order of integrations. Introducing auxiliary fields allows one to do the path

integration over the original fields exactly while holding the auxiliary fields constant. Then one does the remaining path integrations by the method of steepest descent and obtains a loop expansion in terms of the auxiliary-field propagators.

In utilizing the Hubbard-Stratonovich transformation we impose the following requirements: (i) to treat the normal and anamolous densities on an equal footing and (ii) to reduce in the weak-interaction limit to Bogoliubov's theory of interacting bosons (see [24, 25] for reviews). To insure this latter feature we introduce the normal and pairing density composite fields χ_0 and A representing $\sqrt{2}\lambda\phi^*(x)\phi(x)$ and $\lambda\phi(x)\phi(x)$ with the corresponding fluctuations, the Lagrangian density in the LOAF theory becomes [12, 13]

$$\mathcal{L} = \mathcal{L}_0 + [A(x)[\phi^*(x)]^2 + A^*(x)[\phi(x)]^2] -$$
$$\sqrt{2}\chi_0(x)|\phi(x)|^2 + \frac{1}{2\lambda}[\chi_0^2(x) - |A(x)|^2]. \quad (3)$$

Here $\mathcal{L}_0$ denotes the kinetic energy part of Eq. (1). Note that the pairing density field emerges from the pairing channel in Eq. (1). These auxiliary fields introduce composite-field propagators and the counting of their loops facilitates a resummation scheme similar to the large-N expansion [13–16].

The leading-order auxiliary-field (LOAF) theory of 3D Bose gases has been discussed in Ref. [12, 13] and here we briefly review its derivation for a 2D Bose gas. We begin with the Lagrangian density after introducing the composite fields χ_0 and A as shown in Eq. (3). To simplify our expressions, we define $\Phi = (\phi, \phi^*, \chi_0, A, A^*)^T$ and its corresponding source term $J = (j, j^*, s, \tilde{S}, \tilde{S}^*)^T$. The generating functional $W[J]$ can be obtained from the partition function by

$$Z[J] = e^{iW[J]/\hbar} = \mathcal{N}\int \mathcal{D}\Phi e^{(i/\hbar)[S[\Phi] + \int J^\dagger\Phi]},$$
$$S[\Phi] = \int dt d^2x \mathcal{L}. \quad (4)$$

We note here that if we first perform the Gaussian path integration over the auxiliary fields χ_0, A, A^*, we recover the original generating functional based on the Lagrangian density (1). Instead we will reverse the orders of integrations and perform the (now) Gaussian integration over the fields ϕ, ϕ^*. This is the gist of the Hubbard-Stratanovich transformation. The generating functional of one-particle irreducible (1-PI) graphs $\Gamma[\Phi]$ is the Legendre transformation of $W[J]$:

$$\Gamma[\Phi] = \int d^dx J^\dagger(x)\Phi(x) - W[J]. \quad (5)$$

The action $S[\Phi]$ in Eq.(4) written in terms of the auxiliary fields A and χ_0 is quadratic in the fields ϕ, ϕ^*, so that the Gaussian integral in ϕ, ϕ^* can be done exactly, leaving an effective action $S_{eff}[\chi_0, A, A^*]$ which now depends on J, χ_0, A, A^*. In order to perform the remaining integrals we introduce a small parameter ϵ into the problem by replacing $S_{eff} \to S_{eff}/\epsilon$. This allows us to perform the remaining integrals via Laplace's method or the stationary-phase approximation. As shown in Refs. [13, 26], the parameter ϵ counts the number of composite-field (χ and A) propagator loops. The LOAF approximation is the leading order in ϵ and consists of

just keeping the contribution at the stationary phase point. The details of this expansion are given in Ref. [13].

The Legendre transform of the stationary phase approximation for $Z[J]$ is then found to be

$$\Gamma[\Phi] = \frac{1}{2} \int d^dx d^dx' \phi_a^* G_{ab}^{-1}(x,x') \phi_b(x')$$
$$- \int d^dx \left(\frac{\chi_0^2 - |A|^2}{2\lambda} - \frac{\hbar}{2i} \text{Tr}\{\ln[G^{-1}(x,x)]\} \right).$$

Here $G^{-1}(x,x') = \delta(x,x')\tilde{G}^{-1}$ and $\tilde{G}^{-1}$ is given by

$$\begin{pmatrix} -i\hbar\partial_t - \hbar^2\nabla^2/(2m) + \chi & -A \\ -A^* & i\hbar\partial_t - \hbar^2\nabla^2/(2m) + \chi \end{pmatrix}.$$

Here $\chi = \sqrt{2}\chi_0 - \mu$. The effective potential can be evaluated by a Wick rotation to the imaginary time $\tau \rightarrow it$ and using the standard Matsubara frequency summation. For homogeneous static fields we define the effective potential $V_{eff} \equiv \Gamma[\Phi]/\mathcal{V}\beta$, where $\mathcal{V}$ is the volume of the system and $\beta = 1/(k_B T)$. The inverse Green's function becomes

$$G^{-1} = \begin{pmatrix} -i\omega_n + \epsilon_k + \chi & -A \\ -A^* & i\omega_n + \epsilon_k + \chi \end{pmatrix}.$$

Here ω_n is a bosonic Matsubara frequency and $\epsilon_k = \hbar^2 k^2/(2m)$. The last term in V_{eff} is $\frac{1}{2\beta}\text{Tr}\{\ln G^{-1}\} = \frac{1}{2}\sum_k \frac{1}{\beta}\sum_n \ln(\omega_n^2 + \omega_k^2) = \sum_k [(\omega_k/2) + (1/\beta)\ln(1 - e^{-\beta\omega_k})]$. Here $\omega_k = \sqrt{(\epsilon_k + \chi)^2 - |A|^2}$. Then one obtains the expression for the (unrenormalized) effective potential

$$V_{eff} = \chi|\phi|^2 - \frac{A^*\phi^2}{2} - \frac{A(\phi^*)^2}{2} - \frac{(\chi+\mu)^2}{4\lambda} + \frac{|A|^2}{2\lambda} +$$
$$\sum_k \left[\frac{\omega_k}{2} + \frac{1}{\beta}\ln(1 - e^{-\beta\omega_k}) \right]. \quad (6)$$

At the minimum of the potential $\delta V_{eff}/\delta\phi^* = 0$ which leads to the condition $\chi\phi - A\phi^* = 0$. Thus if the minimum is not at $\phi = 0$, we can use the $U(1)$ symmetry to make ϕ and A real and then we obtain in that case $\chi = A$. Indeed, at $T = 0$ the minimum is not at zero and the single-particle Bose-Einstein condensation (BEC) corresponds to a finite $\phi = \sqrt{\rho_0}$. Therefore in the presence of the single-particle BEC, $\chi = A$ and the dispersion is gapless $\omega_k = \sqrt{\epsilon_k(\epsilon_k + 2\chi)}$, where χ plays the role of $\lambda\rho_0$ in the Bogoliubov theory of weakly interacting bosons.

A. Renormalization of LOAF theory

So far the theory has not been renormalized and it is ultraviolet divergent. In Popov's approach to 2D Bose gases [10, 27] a high-energy cutoff has been introduced and this cutoff remains in the equations of state. Here we systematically renormalize the coupling constant, chemical potential, and vacuum energy so that there is no ultra-violet divergence in our theory. By examining V_{eff} shown in Eq. (6) one can see that the

ultraviolet divergence comes from the integral of ω_k. The ultraviolet divergent part of ω_k at large k is $\epsilon_k + \chi - |A|^2/(2\epsilon_k)$ in both 3D and 2D. In 3 D one can relate these terms to usual renormalizations evaluated at $\Omega = q = 0$, where $\hbar\Omega$ and q are the energy transfer and momentum transfer of two-body scattering. In two dimensions, however, one needs to define the renormalized coupling constant at a finite value of Ω and/or q since the scattering amplitude vanishes at zero Ω and q [10, 22].

In our resummed theory the renormalized running coupling constant is defined as the inverse of the second derivative of the effective action with respect to the field A. This leads to an equation

$$\frac{1}{\lambda_R(q,\Omega,T)} = 2D_{AA^*}^{-1}(q,\Omega,T). \quad (7)$$

The inverse AA^* propagator can be obtained by $\delta^2\Gamma[\Phi]/\delta A \delta A^*$. Explicitly,

$$D_{AA^*}^{-1}(x,x',T) = \frac{\delta(x-x')}{2\lambda} + \frac{1}{2}\frac{\delta^2\text{Tr}\ln[G^{-1}]}{\delta A(x)\delta A^*(x')}. \quad (8)$$

After a Fourier transform this becomes

$$D_{AA^*}^{-1}(q,\Omega,T) = \frac{1}{2\lambda} - \frac{1}{2}\Pi(q,\Omega,T). \quad (9)$$

Here $\Pi(q,\Omega,T)$ is the bubble diagram discussed in Ref. [19]. The divergent part of $\Pi(q,\Omega = 0,T = 0)$ in 2D is $(1/2\pi)\int dkk[\sqrt{\epsilon_k^2 + (\epsilon_q/2)^2}]^{-1}$. We define the physical renormalized coupling constant in 2D as the running coupling constant at $T = 0, \Omega = 0, q = q_0$ (of course we can choose any other scale to define the renormalized coupling constant). For a comparison with the relativistic case, one can refer to Ref. [28] and references therein.

We define an intermediate renormalized coupling constant by just keeping the ultraviolet divergent part of the bubble diagram.

$$\frac{1}{\lambda_R(q_0)} = \frac{1}{\lambda} - \int \frac{dkk}{2\pi}\frac{1}{\sqrt{\epsilon_k^2 + (\epsilon_{q_0}/2)^2}}. \quad (10)$$

In terms of this intermediate renormalized coupling constant (which we will choose to be our definition of the renormalized coupling constant λ_R) one finds that the running coupling constant at any scale is given by

$$\frac{1}{\lambda_R(q,\Omega,T)} = \frac{1}{\lambda_R(q_0)} - (\Pi(q,\Omega,T) -$$
$$\int \frac{dkk}{2\pi}\frac{1}{\sqrt{\epsilon_k^2 + (\epsilon_{q_0}/2)^2}} \Bigg). \quad (11)$$

In three dimensions one is allowed to set $q_0 = 0$, since the two-body scattering is finite at zero momentum transfer.

The connection between the 2D renormalized running coupling constant and the t-matrix calculations of the 2D scattering amplitude can be seen clearly at $T = 0$. One can show that $\Pi(q,\Omega = 0,T = 0) - \Pi(q_0,\Omega = 0,T = 0) = (1/2\pi)\ln(q/q_0)$ and as a consequence

$$\lambda_R(q,\Omega = 0,T = 0) = \frac{\lambda_R(q_0)}{1 - \frac{1}{2\pi}\ln\left(\frac{q}{q_0}\right)}. \quad (12)$$

Therefore $\lambda_R(q, \Omega = 0, T = 0) \to 0$ as $q \to 0$, which is consistent with the finding that the 2D scattering amplitude vanishes at zero energy- and momentum- transfer [10, 22] in the t-matrix calculations. This analysis justifies our choice of a finite momentum transfer in defining the running coupling constant. The 2D scattering amplitude at a small momentum transfer is given by $f^{2D} \sim 4\pi/[m|\ln(\rho a^2)|]$, where a is the 2D s-wave scattering length [10, 22]. After the coupling-constant renormalization, λ_R may be set to be proportional to f^{2D} and we formally write

$$\lambda_R = \frac{4\pi\hbar^2}{m|\ln(\rho a^2)|}. \qquad (13)$$

Here a is the scattering length measured at the momentum transfer q_0 and $T = 0$. We focus on the regime $\rho a^2 < 1$, which is consistent with the requirement of a dilute gas. This less restrictive condition, when compared to the condition $|\ln|\ln(\rho a^2)|| \ll 1$ for those perturbative methods reviewed in Ref.[10], allows us to explore intermediate-coupling regimes where $|\ln(\rho a^2)|^{-1} \sim O(1)$.

In contrast to the renormalization of the coupling constant, the chemical-potential and vacuum-energy renormalizations are found to have the same form in two and three dimensions. The chemical-potential renormalization is

$$\frac{\mu_R}{\lambda_R} = \frac{\mu}{\lambda} - \sum_k 1, \qquad (14)$$

The vacuum-energy renormalization is given by

$$V_R - \frac{\mu_R^2}{4\lambda_R} = V_0 - \frac{\mu^2}{4\lambda} - \sum_k \frac{\epsilon_k}{2}, \qquad (15)$$

Here V_0 and V_R are the bare and renormalized vacuum energy.

The LOAF theory written in terms of the renormalized parameters is thus given by

$$V_{eff} = \chi|\phi|^2 - \frac{A^*\phi^2}{2} - \frac{A(\phi^*)^2}{2} - \frac{(\chi+\mu)^2}{4\lambda} + \frac{|A|^2}{2\lambda} + \frac{1}{2\pi}\int_0^\infty dk\, k \left[\frac{\omega_k - \epsilon_k - \chi + \frac{|A|^2}{2\sqrt{\epsilon_k + (\epsilon_{q_0}/2)^2}}}{2} + \frac{1}{\beta}\ln(1 - e^{-\beta\omega_k}) \right]. \qquad (16)$$

Here we drop the index R and the vacuum energy and use continuity to extend our renormalization procedure to the region where $\chi \neq A$. The equations of state are given by $\delta V_{eff}/\delta\chi = 0$, $\delta V_{eff}/\delta A^* = 0$, and $-\delta V_{eff}/\delta\mu = \rho$, which are explicitly shown in the main text.

The LOAF theory then only keeps the leading order terms and one obtains the equations of state (EOS) by minimization of the renormalized V_{eff}:

$$\frac{A}{\lambda} = \rho_0 + A\int \frac{d^2k}{(2\pi)^2}\left[\frac{1 + 2n(\omega_k)}{2\omega_k} - \frac{1}{2\sqrt{\epsilon_k^2 + (\epsilon_{q_0}/2)^2}} \right];$$

$$\rho = \rho_0 + \int \frac{d^2k}{(2\pi)^2}\left[\frac{\epsilon_k + \chi}{2\omega_k}[1 + 2n(\omega_k)] - \frac{1}{2} \right]. \qquad (17)$$
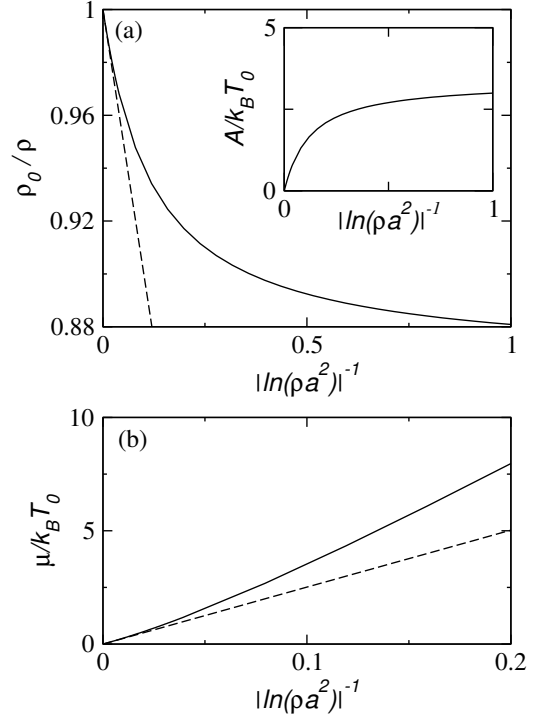

Figure 1. (a) The condensate fraction as a function of $|\ln(\rho a^2)|^{-1}$ at $T = 0$ (solid line). The dashed line shows the prediction from Eq. (19). The inset shows the pairing density field A as a function of $|\ln(\rho a^2)|^{-1}$. (b) The chemical potential as a function of $|\ln(\rho a^2)|^{-1}$ at $T = 0$ (solid line). The dashed line shows the prediction from Eq. (18).

Here $\chi = \sqrt{2}\chi_0 - \mu$, $\omega_k = \sqrt{(\epsilon_k + \chi)^2 - |A|^2}$, $n(x) = 1/(e^{\beta x} - 1)$ is the Bose distribution function, and $\rho_0 = \phi_0^2$ is the condensate density, where ϕ_0 denotes the expectation value of ϕ. The density is related to the chemical potential via $\rho = (\chi + \mu)/2\lambda$. In addition to the EOS, there is a BEC condition $\chi\phi - A\phi^* = 0$. We define $k_0^2 = \rho$, $E_0 \equiv \hbar^2 k_0^2/2m \equiv k_B T_0$ and use k_0, E_0, and T_0 as our units with $k_B \equiv 1$. The quantity q_0 is the scale that one defines the running coupling constant $\lambda(q, \Omega, T)$ in a 2D Bose gas. It also defines the momentum transfer at which the scattering length a is measured. We emphasize again that in 2D q_0 cannot be chosen to be zero due to the peculiar behavior of the scattering amplitude. However, this choice of scale does not effect any physically measurable quantities as argued in standard renormalization methods [15]. Here we choose $q_0/k_0 = 0.1$. To compare with experimental parameters, one only needs to find out the momentum transfer q_0 at which the relation $f^{2D} \sim 4\pi/[m|\ln(\rho a^2)|]$ is defined. That q_0 then serves as the renormalization energy scale in the EOS.

At $T = 0$ the LOAF theory predicts a finite ρ_0 and BEC. Moreover, the BEC condition $\chi\phi - A\phi^* = 0$ requires that $\chi = |A|$ so that $\omega_k = \sqrt{\epsilon_k(\epsilon_k + 2\chi)}$ is gapless. This gapless excitation is associated with the Goldstone mode in the BEC phase [19]. The equations of state become $(A/\lambda) = \rho_0 - (A/8\pi)\ln(2A/\epsilon_{q_0})$ and $\rho = \rho_0 + A/8\pi$. Figure 1 (a) shows that ρ_0/ρ decreases and $A/k_B T_0$ increases as the

interaction $|\ln(\rho a^2)|^{-1}$ increases. The chemical potential is shown in Figure 1 (b). The condensate fraction and the chemical potential from perturbative calculations [29] are given by

$$\mu = \frac{4\pi\hbar^2\rho}{m|\ln(\rho a^2)|}[1 + O(|\ln(\rho a^2)|^{-1})], \qquad (18)$$

$$\frac{\rho_0}{\rho} = 1 - \frac{1}{|\ln(\rho a^2)|} + O(|\ln(\rho a^2)|^{-2}). \qquad (19)$$

The dashed lines in Figure 1 show the results from perturbative calculations. One can see that for extremely small $|\ln(\rho a^2)|^{-1}$, the LOAF theory agrees well with the perturbative calculations. Thus the LOAF theory agrees quantitatively with perturbation theory results and should be reliable in the weakly interacting regime. Importantly, the LOAF theory could help explore interesting physics beyond the weakly interacting regime.

B. Phase fluctuations

At finite T, Mermin-Wagner theorem [21] rules out the possibility of long-range orders so BEC cannot survive. In other words, the $U(1)$ symmetry of the Lagrangian density 1 should remain unbroken at any finite T. The lack of a broken symmetry implies that a gapless Goldstone mode should not exist and the excitation should be gapped. This is consistent with Eq. (17) since the equations cannot be satisfied by a gapless dispersion. In the LOAF theory this indicates that the BEC condition cannot be met so ρ_0 must vanish. Eq. (17), however, does not rule out the possibility of a finite A and indeed we found finite values of A at finite T. The finite expectation value of A implies a diatomic condensate, which also could break the $U(1)$ symmetry of the Lagrangian density (1) [19] and violate the Mermin-Wagner theorem.

This apparent conflict was analyzed in great detail by Witten [30] in the $SU(N)$ Thirring model at large-N. His arguments would lead here to the conclusion that there is a gapless mode associated with the phase of A but that this will *not* be a Goldstone mode. He also argues that apart from the fact that there is no symmetry breaking at finite T, the fermions (which in our case will be the boson ϕ) will have an energy gap in the phase-disordered regime and that apart from the details of the BKT phase transition [31], the large-N predictions (which are similar in spirit to the LOAF theory) are quite reliable.

In the BCS theory of attractive fermions, the method of obtaining a BKT transition in 2D by introducing phase fluctuations to disorder the would-be order parameter has been discussed in Refs. [7, 11]. There after obtaining the BCS theory at the mean-field level, one further introduces a phase for the gap which is the analogue of the anomalous condensate present in the LOAF theory. It has been shown that the BCS theory can be derived from the same LOAF framework [32] and one can obtain similar Josephson relations in both the BCS theory of attractive fermions and the LOAF theory of repulsive bosons [20]. Therefore phase fluctuations may be incorporated into the LOAF theory of bosons using a method similar to that for the BCS theory of attractive fermions.

Following the phase-fluctuation method of the Thirring model and the BCS theory, we introduce phase fluctuations into the solution of the EOS of the LOAF theory [7, 11, 30]. This procedure also introduces the BKT transition to our theory and determines where the superfluid phase is stable. The idea is to include a fluctuating phase in the pairing density field so it becomes $Ae^{i\theta}$. As discussed in Ref. [20], the phase of the pairing field is twice of the phase of the bosonic field and both phases originate from the $U(1)$ symmetry of the Lagrangian density (1). The amplitude A is determined by the EOS, Eq. (17), and can be finite. Similar to Ref. [7] we work with the minimum where A is constant. Following Refs. [7, 30], in the action containing θ we only keep the leading-order contribution of the phase fluctuation, which is proportional to $\int d^2x(\nabla\theta)^2$. This kinetic-energy term of θ corresponds to the XY model and thus the conventional BKT physics [31] is introduced to the theory following the arguments shown in Section 5 of Ref. [7]. The proportionality coefficient of the kinetic-energy term of θ is the phase stiffness, which is equal to the superfluid density $\rho_s = \delta^2 V_{eff}/\delta v\delta v$ following a similar calculation of Ref. [20]. Here $v = \nabla\theta$.

Similar to the results presented in Ref. [7], the phase fluctuations obey $\langle e^{i\theta}\rangle = 0$ and as a consequence, there is no long-range coherence of the pairing density field. The correlation of the phase is $\langle e^{i\theta(\mathbf{x})}e^{i\theta(0)}\rangle \sim |\mathbf{x}|^{-mT/(2\pi\rho_s)}$ below the BKT transition temperature T_{BKT} and $\langle e^{i\theta(\mathbf{x})}e^{i\theta(0)}\rangle \sim e^{-|\mathbf{x}|/x_0}$ above T_{BKT}, where x_0 is the characteristic length for the decay of the correlation [31]. The conventional picture is that vortex-antivortex pairs are bound below T_{BKT} and a superfluid phase is possible. Above T_{BKT} vortices and antivortices unbind and proliferate so the superfluid is destroyed. Thus the phase fluctuations introduce a BKT transition separating a low-T superfluid phase and a non-superfluid phase.

III. RESULTS AND DISCUSSIONS

A. Finite-T phase diagram

We now construct the finite-T phase diagram. The pairing onset temperature T_p is determined by the EOS (17) when the amplitude A first becomes finite. Figure 2 (a) shows T_p as a function of η. There is no genuine phase transition across T_p. Below T_p bosons form composite pairing density field but the phase is random. In other words, below T_p there is a *phase-disordered diatomic quasi-condensate*. We note that in the $2+1$-dimensional relativistic $O(N)$ ϕ^4 model, there is a resonance in the $\phi-\phi$ scattering amplitude near twice the mass of the scalar meson at small coupling [28]. Further studies may determine if there is finite two-body binding energy. Fig. 2 (b) shows the growth of the amplitude of A as T decreases.

Next we investigate where superfluidity becomes stable. The method for determining the superfluid transition temperature comes from the analogy with the XY model once one adds the phase fluctuations [7]. According to the theory of BKT transition [31], the superfluid is unstable above T_{BKT} due to vortex-antivortex proliferation, where T_{BKT} is deter-
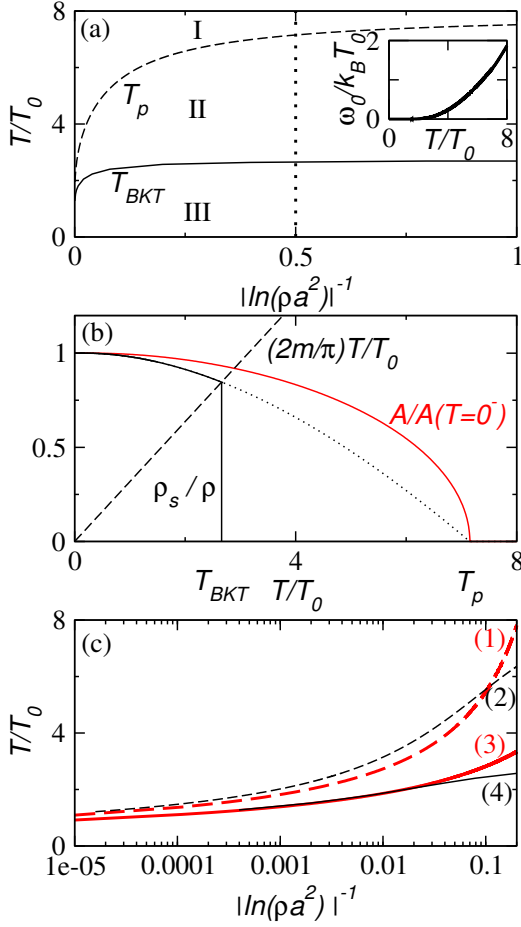
Figure 2. (a) Phase diagram of a 2D Bose gas from the LOAF theory with phase fluctuations. The solid and dashed lines show the BKT and pairing onset temperatures. Regions I, II, and III correspond to the normal, pairing, and superfluid phases. The details of physical quantities along the dotted line ($|\ln(\rho a^2)|^{-1} = 0.5$) are shown in panel (b). Inset: The gap in the dispersion, $\omega_k(k=0) = \omega_0$, as a function of T for $|\ln(\rho a^2)|^{-1} = 0.5$. (b) The amplitude of the pairing density field A and the superfluid fraction ρ_s/ρ as a function of T for $|\ln(\rho a^2)|^{-1} = 0.5$. The dashed line is $(2m/\pi)T/T_0$ and when it intersects the curve of ρ_s/ρ, the BKT transition occurs and the superfluid density drops to zero. (c) Comparison of (1) T_c^{RG} from Eq. (22), (2) T_p from the LOAF theory, (3) T_{BKT} from Eq. (23) with $C = 2.152$, and (4) T_{BKT} from the LOAF theory in the weakly interacting regime.

mined by

$$k_B T_{BKT} = \frac{\pi \hbar^2}{2m} \rho_s(T_{BKT}). \quad (20)$$

The superfluid density ρ_s of the LOAF theory has been discussed in Ref. [19] and it can be obtained from the Landau two-fluid model or the current-current response function. It has been argued that the pairing density field is crucial in sustaining a finite ρ_s. This feature is similar to the fermionic BCS theory, where the superfluidity comes from Cooper pairs.

When $\rho_0 = 0$ but $A > 0$, one has [19]

$$\rho_s = \rho - \frac{\hbar^2}{m} \int \frac{d^2k}{(2\pi)^2} \left(\frac{k^2}{2} \right) \left(-\frac{\partial n(\omega_k)}{\partial \omega_k} \right). \quad (21)$$

Fig. 2 (b) shows ρ_s/ρ as a function of T for $|\ln(\rho a^2)| = 0.5$. When this curve intersects the line of $(2m/\hbar^2\pi)T/T_0$, the BKT condition (20) is met and vortex-antivortex proliferation will destroy the superfluidity above T_{BKT}. As a consequence, ρ_s jumps to zero and the superfluid phase is only stable below T_{BKT}.

Following this procedure we show T_{BKT} as a function of $|\ln(\rho a^2)|^{-1}$ in Fig. 2 (a). There is a genuine phase transition across T_{BKT} since the superfluid density is discontinuous across this boundary. We therefore identify three different phases of a 2D Bose gas at finite T as shown on Fig. 2 (a): Regime I above T_p corresponds to a normal gas with no pairing density nor superfluidity. Regime II in between T_{BKT} and T_p is a non-superfluid phase with a finite amplitude of the pairing density field but no phase coherence. Regime III below T_{BKT} is a superfluid phase with algebraically decaying phase correlations. One can see that T_p is about $2-3$ times of T_{BKT} and is not a high-temperature scale as one may inferred from Ref. [1]. In the LOAF theory, the phase diagrams at fixed values of $|\ln(\rho a^2)|^{-1}$ are similar to the one shown in Fig. 2 (b) (i. e., the amplitude of A smoothly approaches zero at T_p while ρ_s drops to zero at T_{BKT}) but with different values of T_p and T_{BKT} which can be inferred from Fig. 2. (a).

The superfluid transition temperature in the weakly interacting regime has been theoretically studied in previous work (see [10] for a review). In Ref. [33] a renormalization-group approach predicts that

$$T_c^{RG} \sim \frac{2\pi\rho}{m \ln |\ln(\rho a^2)|}. \quad (22)$$

Monte Carlo simulations in Refs. [34, 35] suggest the functional form

$$T_{BKT} = \frac{2\pi\rho}{m} \frac{1}{C + \ln |\ln(\rho a^2)|}. \quad (23)$$

Fitting T_{BKT} from the LOAF theory at weak coupling to the functional form of Eq. (23) leads to the results shown in Figure 2. From the fitting we obtain $C = 2.152$ as compared with the Monte Carlo result of Ref. [35], which yielded the numerical value $C = 3.409$ [36]. Figure 2(c) shows T_p and T_{BKT} from the LOAF theory along with T_c^{RG} and T_{BKT} from Eq. (23) with a constant $C = 2.152$ in the weakly interacting regime. One can see that the LOAF theory predicts a T_{BKT} that agrees well with the functional form suggested by Monte Carlo simulations when $|\ln(\rho a^2)|^{-1} < 0.01$. In contrast, T_c^{RG} seems to agree with T_p when the interaction strength is extremely small. Moreover, T_p and T_{BKT} from the LOAF theory approach each other as $|\ln(\rho a^2)|^{-1}$ approaches zero. As the interaction becomes stronger, T_{BKT} as obtained from the LOAF theory starts to deviate from T_{BKT} from Eq. (23) and remains smaller than both T_c^{RG} and Eq. (23). The double logarithmic behavior of both T_p and T_{BKT} from

the LOAF theory in the weakly interacting regime also suggests that our theory captures the qualitative features of both Monte Carlo and renormalization-group results. LOAF theory serves as an extrapolation beyond weak coupling and provides predictions that can be compared with experiments.

Interestingly, the phase diagram of Fig. 2 (a) is similar to the phase diagram of a 2D Fermi gas with attractive interactions [11]. There are subtle differences [37]. For example, T_{BKT} for fermions increases as the attractive interactions increase but for bosons it increases as the repulsion increases. The slow increase of T_{BKT} as a function of $|\ln(\rho a^2)|^{-1}$ away from the weakly interacting regime agrees qualitatively with more recent Monte Carlo simulations [38].

B. Other experimental implications

We now address the issue whether a finite amplitude of the pairing density field results in any observable effects. One observable signature is a gapped excitation energy spectrum $\omega_k = \sqrt{(\epsilon_k + \chi)^2 - |A|^2}$ at finite T (consistent with the analysis of Ref. [30]), which is different from the gapless Bogoliubov spectrum. The inset of Fig. 2 (a) shows the gap $\omega_k(k = 0)$, which is finite and increasing as T increases. The dispersion may be measured using Bragg scattering [39]. Another possible signature may be revealed by the analogue of radio-frequency (RF) spectroscopy, which shows the potential of measuring the spectral function, or equivalently, the imaginary part of the single-particle Green's function [40]. For fermions with attractive interactions, the spectral function of a homogeneous gas could show a two-peak structure due to the particle-hole mixing in the formation of Cooper pairs [40]. Here we investigate if there is a similar structure for bosons.

The single-particle Green's function from the LOAF theory is [19]

$$G_{MF}(k, i\omega_n) = \frac{i\omega_n + \epsilon_k + \chi}{\omega_n^2 + \omega_k^2}. \qquad (24)$$

Here ω_n is the bosonic Matsubara frequency. Making the analytic continuation $i\omega_n \to \omega + i0^+$, one obtains $G_{MF}(k, \omega)$ [18]. The spectral function is defined as $\mathcal{A}(k, \omega) = 2\mathrm{Im}G(k, \omega)$, where $G(k, \omega)$ is the single-particle Green's function of a given theory, and it satisfies the sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathcal{A}(k, \omega) = 1 \qquad (25)$$

for any T.

The LOAF theory predicts a qualitative difference in the spectral function when the amplitude of A becomes finite. Below T_p, one has $\omega_k = \sqrt{(\epsilon_k + \chi + A)(\epsilon_k + \chi - A)}$ and $\mathcal{A}(k, \omega) = 2\pi u_k^2 \delta(\omega - \omega_k) - 2\pi v_k^2 \delta(\omega + \omega_k)$. Here $u_k^2, v_k^2 = [(\epsilon_k + \chi)/\omega_k \pm 1]/2$. This expression implies that there are two peaks at $\omega = \pm\omega_k$ for a fixed k. This is in contrast to the spectral function in regime I where $A = 0$. In regime I, $\omega_k = \epsilon_k + \chi$ so the spectral function is $\mathcal{A}(k, \omega) = 2\pi\delta(\omega - \omega_k)$. There is only one peak in the spectral function in the normal phase.

The different numbers of peaks in the spectral function below and above T_p is a prediction from the LOAF theory. The delta-function peaks are due to the fact that only the leading-order contributions from the composite fields are included at the mean-field level. To obtain the widths of the spectral peaks, one has to go beyond the leading-order theory. For the relativistic ϕ^4 theory it has been shown in Ref. [41] that by considering a self-consistent ϵ expansion for the generating functional of the two-particle irreducible graphs, one obtains an approximation to the coupled Green fuinction equations which generate a finite imaginary part in the self energy and as a consequence the spectral peaks will be broadened.

In particular, above T_p when $A = 0$, our theory beyond the leading order can be formulated as a set of Schwinger-Dyson (SD) equations following Ref. [41]

$$G^{-1} = G_{MF}^{-1} + \Sigma,$$

$$\Sigma = \int G\mathcal{D}\Lambda,$$

$$\mathcal{D}^{-1} = \mathcal{D}_0^{-1} + \Pi,$$

$$\Pi = \int GG\Lambda. \qquad (26)$$

Here Σ is the self energy of bosons, $\mathcal{D}$ is the composite-field propagator, Λ is the interaction vertex, $D_0^{-1}(x, x') = \delta(x - x')/\lambda$ is the inverse bare composite-field propagator, Π is the self energy of composite fields. To lowest order one may use the approximation $\Lambda = 1$, $\mathcal{D} = \mathcal{D}_0$, $G = G_{MF}$, and $\Pi = \Pi_0 = \int G_{MF}G_{MF}$ on the right-hand side. By writing $\Sigma = \mathrm{Re}\Sigma + i\mathrm{Im}\Sigma$, one can see that the delta function in the spectral function is replaced by a Lorentzian function with a full width at half maximum equal to $2\mathrm{Im}\Sigma$. Below T_p there are two finite composite fields, A and χ, and the Green's functions of ϕ, χ, and A are mixed to form a 5×5 matrix $G_{\alpha\beta}$, where $\alpha, \beta = 1, \cdots, 5$ corresponding to $(\phi, \phi^*, \chi, A, A^*)$. Following Ref. [41], the SD equations are

$$G_{\alpha\beta}^{-1} = G_{MF,\alpha\beta}^{-1} + \Sigma_{\alpha\beta},$$

$$\Sigma_{\alpha\beta} = \int \lambda_{\alpha\alpha'\beta'} G_{\alpha'\alpha''} G_{\beta'\beta''} \Lambda_{\alpha''\beta''\beta},$$

$$\Lambda_{\alpha\beta\gamma} = \lambda_{\alpha\beta\gamma} - \frac{\delta\Sigma_{\alpha\beta}}{\delta\phi_\gamma}. \qquad (27)$$

Here repeated indices are summed, $\lambda_{\alpha\beta\gamma}$ is the bare vertex function, and ϕ_γ is an element of $(\phi, \phi^*, \chi, A, A^*)$. One may implement further approximations such as the bare-vertex approximation and resort to numerical methods for evaluating the Green's function beyond the mean-field level as discussed in Ref. [41].

Instead of performing these intricate numerical calculations that should only lead to quantitative corrections, here we focus on the qualitative features of the spectral function already present in the mean-field level but modified by the broadening of the higher-order corrections. The delta functions in $\mathcal{A}(k, \omega)$ evaluated from G_{MF} will be broadened by effects beyond the LOAF theory and for illustrative purposes only, we introduce a Lorentzian function by $\delta(x) \to (\frac{1}{\pi})\frac{\Gamma/2}{x^2 + (\Gamma/2)^2}$ to approximate the spectral peaks. The width Γ could be obtained from
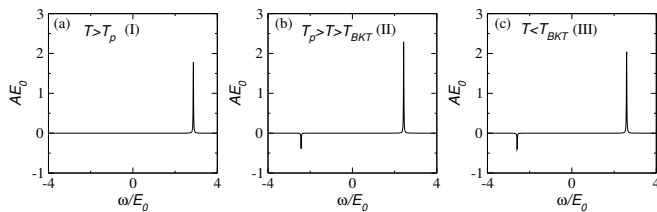
Figure 3. Spectral functions at fixed $k = k_0$ for (a) $T > T_p$ ($T/T_0 = 8$), (b) $T_p > T > T_{BKT}$ ($T/T_0 = 4$), and (c) $T < T_{BKT}$ ($T/T_0 = 1.3$). They belong to regimes I, II, and III of Fig. 2 (a), respectively. Here $|\ln(\rho a^2)|^{-1} = 0.5$.

the full expression of the self energy Σ outlined above, but here for simplicity we set $\Gamma/E_0 = 0.02$. A fully numerical calculations similar to the $T = 0$ calculations in Ref. [42] may help determine the dependence of Γ on T and the interaction strength. Our approximation of the delta function still respects the sum rule (25) for $\mathcal{A}(k, \omega)$. Figure 3 shows the spectral function $\mathcal{A}(k, \omega)$ at fixed $k = k_0$ for three selected temperatures corresponding to regimes I, II, and III of Fig. 2.

When $T > T_p$, $A = 0$ so there is only one peak as shown in Fig. 3(a). Below T_p the finite amplitude of the pairing density field induces another peak in the negative energy region. In the Bogoliubov theory of weakly interacting bosons, the Bogoliubov transformation mixes the creation and annihilation operators. Since the LOAF theory is a natural generalization of the Bogoliubov theory, the pairing density field includes similar mixing effects. Thus the spectral weights of positive and negative energy states are correlated. The two-peak structure reflects this type of correlation effects. The spectral function of a $T = 0$ 2D Bose gas has been evaluated using numerical functional renormalization group method focusing on the positive-energy peak [42]. Since the single-particle Green's function (24) only contains information about the amplitude of the pairing density field, it does not exhibit observable signatures of the BKT transition (see Fig. 3 (b) and (c)).

We note that the spectral function of a fermionic BCS superfluid is $\mathcal{A}(k, \omega) = \tilde{u}_k^2 \delta(\omega - E_k) + \tilde{v}_k^2 \delta(\omega + E_k)$, where $\tilde{u}_k^2, \tilde{v}_k^2 = [1 \pm (\epsilon_k - \mu)/E_k]/2$, $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$, and Δ is the gap function. When $\Delta > 0$, there are two *positive* peaks reflecting the pairing between fermions. The spin statistics, nevertheless, causes one positive and one *negative* peaks for bosons. We emphasize that although this negative peak should also survive in 3D Bose gases [43], its appearance in 2D Bose gases is a more direct evidence of the many-body pairing effect because the BEC vanishes at finite T.

Spectroscopies probing single-particle excitations such as RF measurements may be sensitive only to the existence of an energy gap but not to phase coherence [40]. From Fig. 2 (b) and Fig. 3 we reach a similar conclusion. To probe the BKT transition and the superfluid phase below it, in addition to Ref. [1] we suggest experiments such as the measurement of the second sound, which has been shown to be an indication of superfluidity using hydrodynamic approaches in both 3D [44] and quasi-1D [45] geometries and should have the same resolution in 2D.

IV. CONCLUSION

In summary, we present a coherent mean-field picture of pairing effects, superfluidity, BKT physics, and single-particle excitations by introducing phase fluctuations into the LOAF theory of a 2D interacting Bose gas in a manner similar to what is done in the 2D BCS theory as well as in the Thirring model. In addition to mapping out the phase diagram at finite T, our theory predicts observable signatures of pairing effects above the BKT transition temperature, which resembles the pseudogap physics of 2D Fermi gases [6]. The LOAF theory agrees reasonably with previous results from perturbative calculations, renormalization-group calculations, and Monte Carlo simulations in the weakly interacting regime but further explores the regime of intermediate interaction strength. By implementing the local density approximation for trapped gases, our theory may provide more insights into experiments such as Refs. [3, 5].

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